

Microcystin LR

101043-37-2 | DTXSID3031654

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 6.82e-02 mol/L

Global applicability domain: Outside

Local applicability domain index: 6.06e-02

Confidence level: 3.99e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Chlorhexidine</div> <div>Measured: 1.58e-03</div> <div>Predicted: 6.11e-03</div>	<div>Image not found</div> <div>Guanidine, N,N'''-(iminodi-8,1-octanediyl)bis-</div> <div>Measured: 2.15</div> <div>Predicted: 9.84e-01</div>	<div>Image not found</div> <div>Azidamfenicol</div> <div>[INN:BAN:DCF]</div> <div>Measured: 6.77e-02</div> <div>Predicted: 2.98e-01</div>
<div>Image not found</div> <div>Sulfaguanidine</div> <div>Measured: 1.03e-02</div> <div>Predicted: 4.21e-02</div>	<div>Image not found</div> <div>Arginine</div> <div>Measured: 1.04</div> <div>Predicted: 7.61e-01</div>	